Electronic Supplementary Information (ESI)

Synthesis of visible-light-absorptive and hole-transporting periodic mesoporous organosilica thin films for organic solar cells

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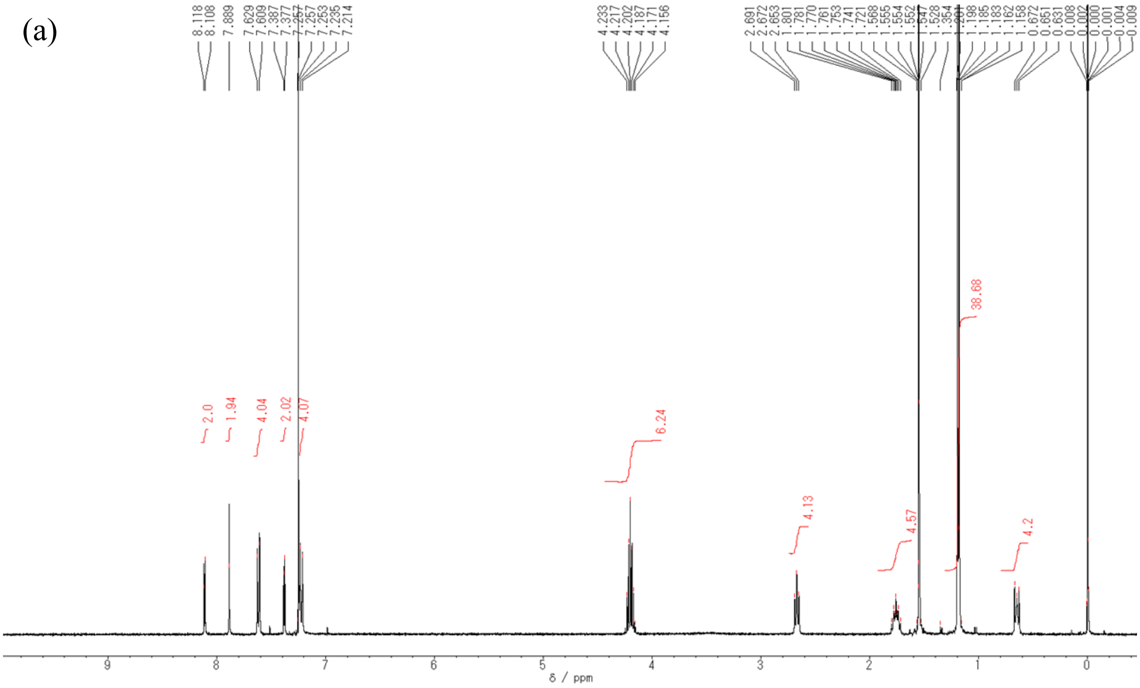
(a)



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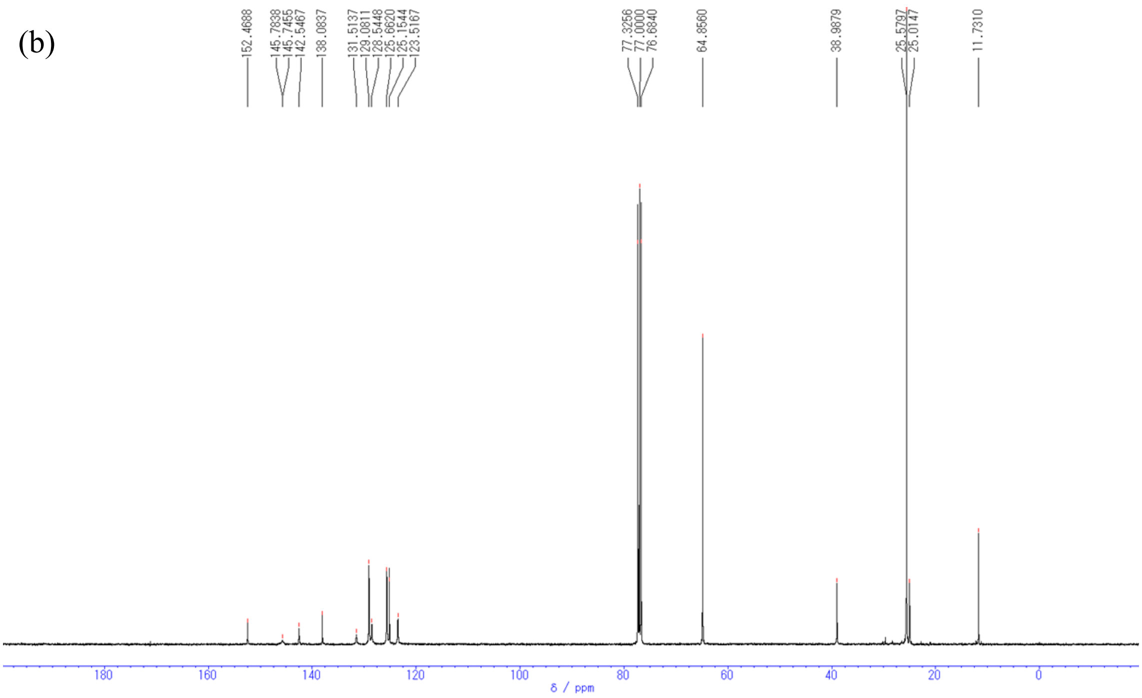
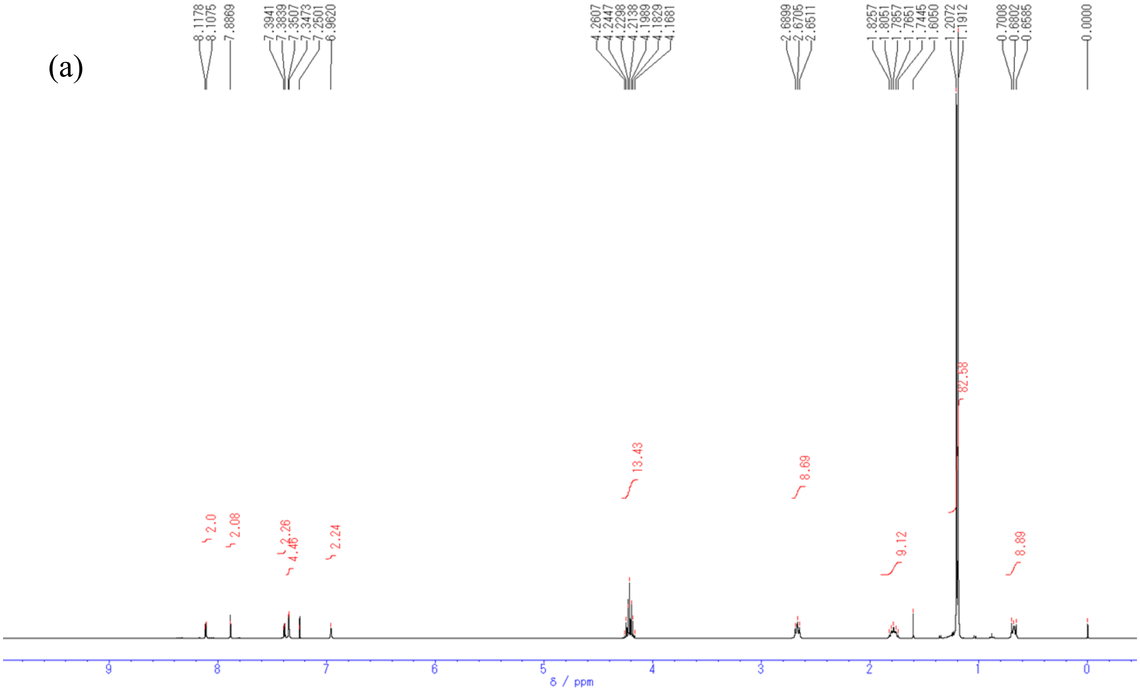


Figure S1. (a) ^{1}H NMR and (b) ^{13}C NMR spectra of organosilane precursor **1** in $CDCl_3$.

(a)



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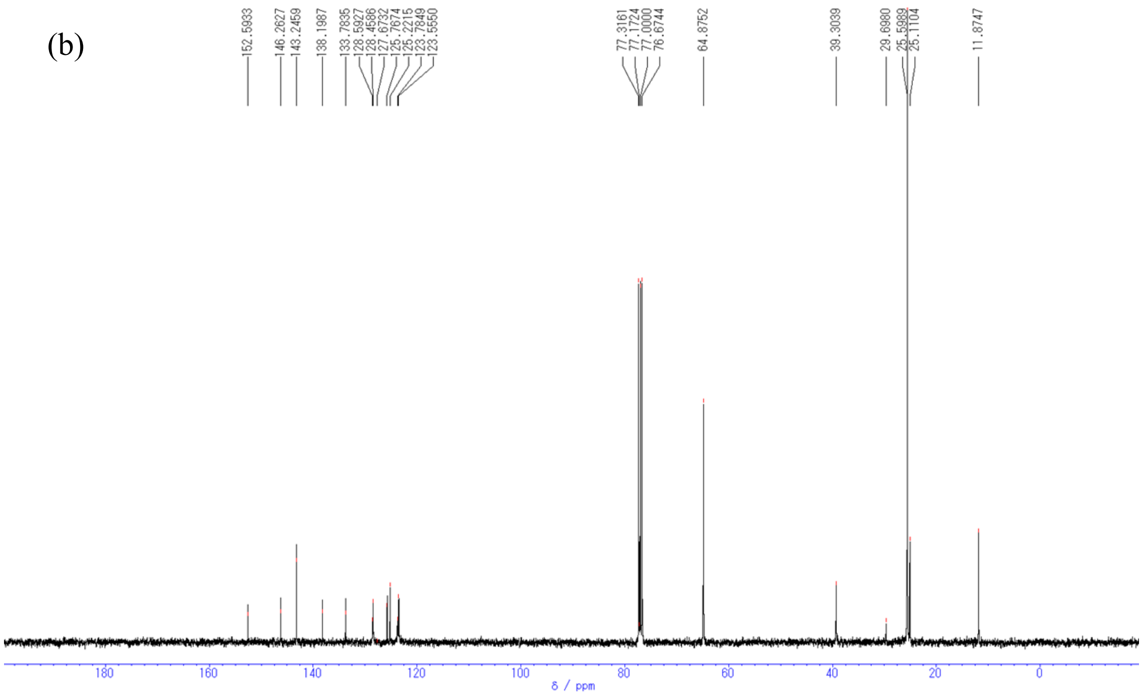


Figure S2. (a) ^{1}H NMR and (b) ^{13}C NMR spectra of organosilane precursor **2** in $CDCl_3$.

Krypton adsorption−desorption isotherms

Krypton adsorption−desorption isotherms were measured using a Quantachrome Autosorb-1 at 87 K. The films (**1-PMO-F**) were formed on 16 cleaned glass substrates (24 mm×32 mm×0.15 mm) by spin-coating sol C and extracting templates. The total weight of **1-PMO-F** (16 peices) was 0.31 mg. The samples were sliced into pieces and placed in a special cell for the measurements of isotherms.

Figure S3 shows a krypton adsorption−desorption isotherm of **1-PMO-F** on glass substrates. The Brunauer−Emmett−Teller (BET) surface area was calculated to be 285 m^2 g^{-1}.

From SEM images of **1-PMO-F**, we estimated the number of mesopores with a diameter of 15 nm to be 18 in a unit cell of (50×50×50) nm^3. Using this information and the weight of **1-PMO-F** measured (0.31 mg), we estimated that the surface area is 225 m^2 g^{-1}. There is no large difference between the value obtained from the experiment and the estimated value.

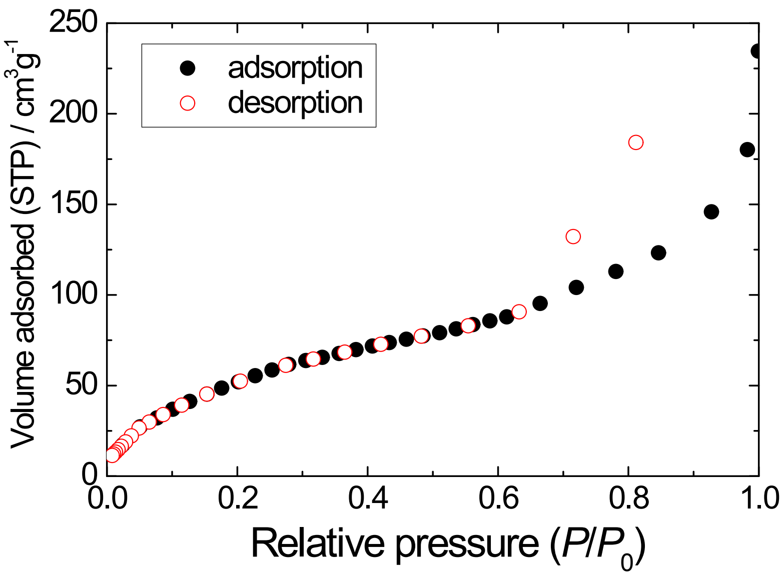


Figure S3. Krypton adsorption−desorption isotherm of **1-PMO-F.**

Pore size distribution of mesopores

We analyzed the pore size distribution for mesopores in top-view SEM images of **1-PMO-F** using an image analysis software. Figure S4 shows pore size distribution of mesopores. Three different SEM images were used (analyzed area: 1.1 μm^2).

From this analysis, we obtained the average pore size for mesopores and its standard deviation. Those values are 15 and 4 nm, respectively. The coefficient of variation (standard deviation / average pore diameter) is about 0.28. The value is similar to that (0.22*) of a conventional PMO film which was estimated by the pore size distribution curve derived from nitrogen adsorption.[16]

(* The value of 0.22 was estimated from inset data of Fig. S7 in ESI (reference 16).)

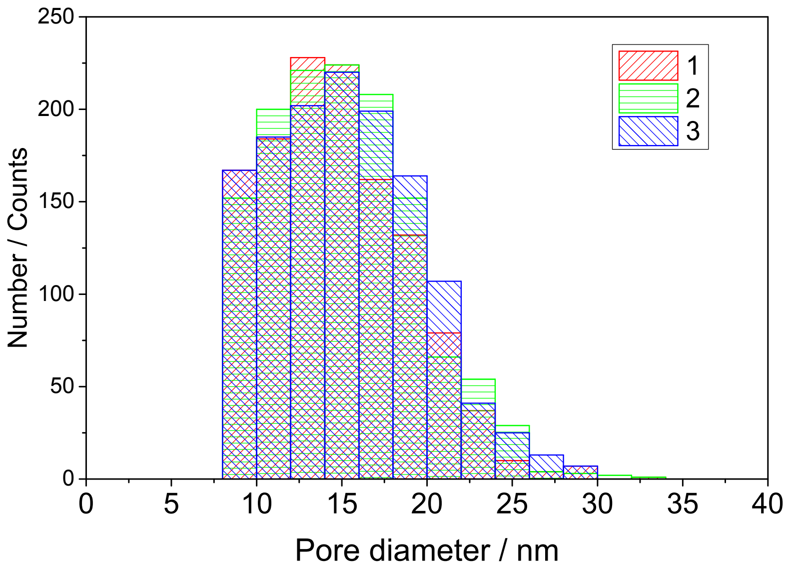


Figure S4. Pore size distribution of mesopores for **1-PMO-F**. Three different Top-view SEM images were analyzed.

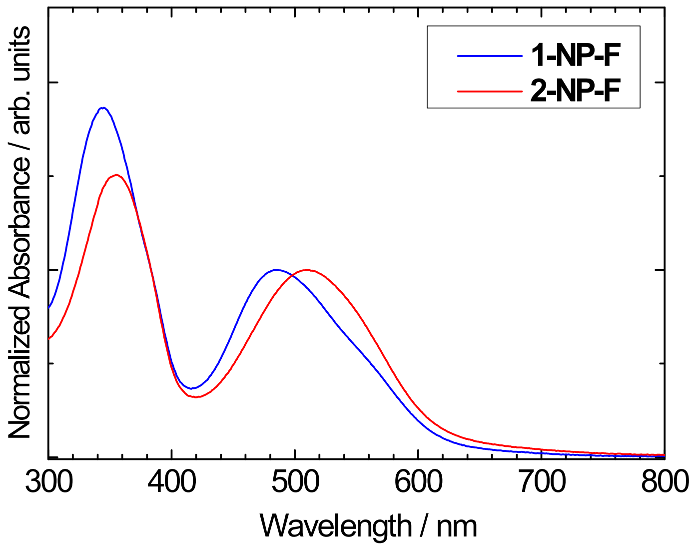


Figure S5. Normalized absorbance of both **1-NP-F** (blue) and **2-NP-F** (red) films.

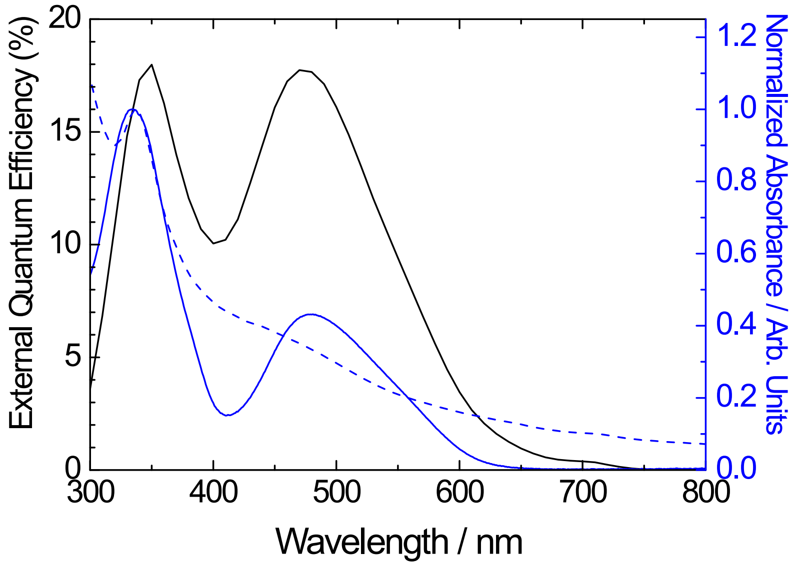


Figure S6. EQE of the **1-PMO-F** based solar cell (black, solid), and normalized absorbance of both **1-PMO-F** (blue, solid) and PCBM (blue, dashed) films.

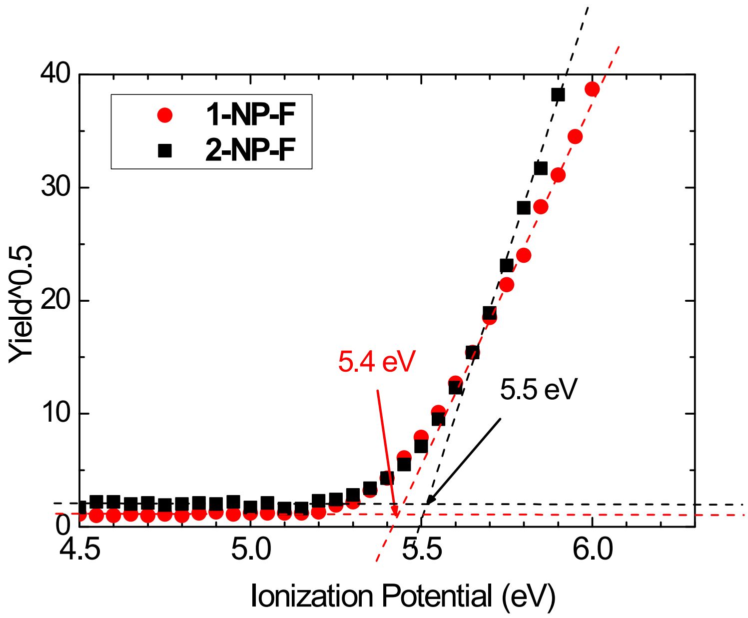
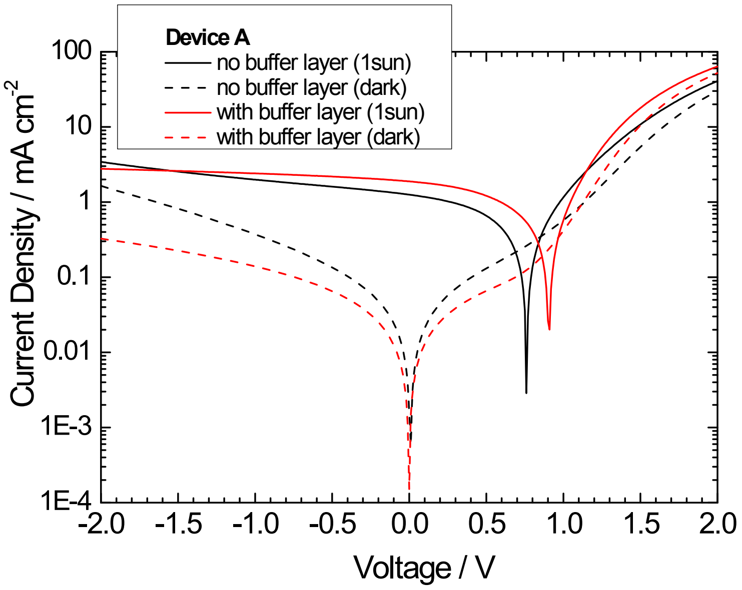


Figure S7. Ionization potentials of **1-NP-F** and **2-NP-F** measured by using AC-2.

(a)



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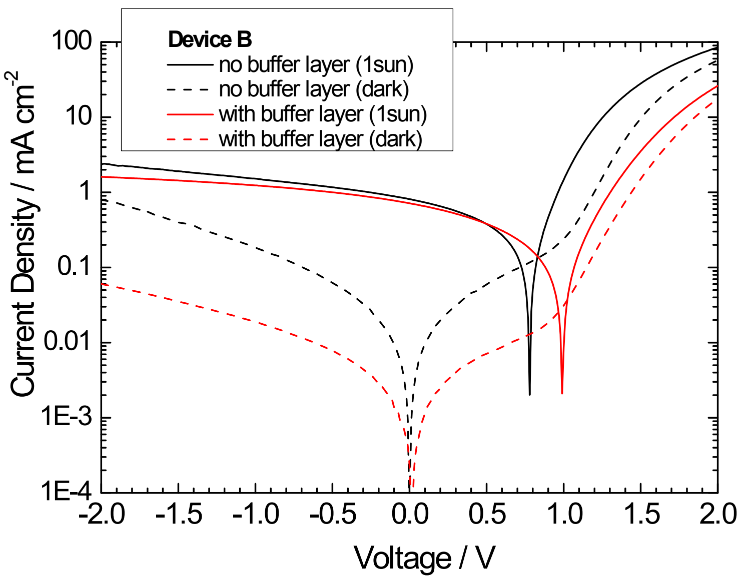

Figure S8. *J*–*V* characteristics of (a) **device A** or (b) **device B** without a buffer layer (black lines) and with **1'-NP-F** buffer layer (red lines) in the dark (broken lines) and under 1 sun, AM1.5 illumination (solid lines).